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TO OUR CUSTOMERS

Dear MICRESS® user,

enclosed please find the most recent release of your MICRESS® software package. The present release 7.0 of MICRESS® comprises a number of improvements and new functionalities. Of course, we also attempted to fix all bugs being reported by our user community.

The present release represents a major version step to version 7.0. The most obvious and most important change is a rearranged input order for the driving file leading to a more user friendly and logical structure. The conversion of “old” driving files to new version 7.0 driving files is supported by MICPad.

Different variants are provided:

- MICRESS® 7.0 is available with or without TQ coupling. The coupled version uses the TQ library corresponding to Thermo-Calc release TC 2019a. GES5 files created with Thermo-Calc version TC 2015b and above are compatible. A new MICRESS®-TQ license file for TQ 2019a is provided along with the current release mail for all users of MICRESS®-TQ with valid maintenance.

- MICRESS® 7.0 is supplied as serial or as partly parallelized version. The solvers for diffusion, stress, flow, temperature and the solver for volume change can be executed multi-threaded based on OpenMP (www.openmp.org).

- MICRESS® 7.0 is supported for Windows (7 and 10) as well as for Linux (Ubuntu 18.04 LTS, CentOS 7, and OpenSUSE 15 Leap). All platforms have to be 64 bit.

Along with MICRESS®, we provide the tools:

- DP_MICRESS 7.123
- MICpad 7.0

DP_MICRESS is also freely available from the MICRESS® website (www.micress.de).

News on MICRESS®:

In detail, the release 7.0 of MICRESS® comprises a number of new functionalities and features as shortly described in the following:

Improvements in input:

- MICRESS® 7.0 comes with an entirely reworked, more logical and more intuitive input file structure. Conversion of old (Version 6.4) driving files is possible via MICpad.

New functionalities:

- As an alternative to the “classical” multiphase-field model, a reformulated version handles volume changes during phase transformations in an approximated manner. This is e.g. essential to simulate graphite growth in cast iron.
- Extended restart-structure-only functionality (with zoom, shift and rotation) now also allows a change of dimensionality, e.g. to extract a 2D section from a 3D simulation. Note that the ‘structure-only’ input has been moved to the initial microstructure block. This block also contains the grain input part.
- Temperature profiles over time can now be used also along with the moving frame option.
- New option "ordered"/"disordered": These criteria can be specified in the "numerical parameters/concentration solver" section and can be used as alternative to "limits" or "criterion_lower/criterion_higher" in cases where an order-disorder transition is possible, like in γ/γ' in Ni-based alloys. The criterion checks whether two sublattices are identical (disordered) or different (ordered).
- The new functionality “split_from_grain” allows for the generation of separated parts of a grain, e.g. during melting. It is the analogue to the "add_to_grain" functionality and a reverse operation to "categorization". It comes as an option in the nucleation data and allows the user to address grain fragments which lost their spatial connection to the main part of the grain e.g. during melting. This function not only allows assigning a new grain number but also to change all the grain data as defined in the corresponding nucleation type (phase, orientation, shield data, etc.).
- New facet, resp. faceted_c, model. The new approach combines the advantages of the two existing models faceted_a and faceted_b and will become standard in the future.
- A new flag "penalty" replaces part of the functionality of the "limits" function in the "stoichiometric phases" input section. It provides a penalty term on the driving force for phase transformations and thus allows for avoiding negative or improper compositions under various circumstances. This new "penalty" function provides more control over the implied phase interaction and also strongly reduces undesired side-effects when using the penalty terms on the driving force.
- The seed density distribution for nucleation can be specified as a log-normal distribution.

Improved functionalities:

- The treatment of eutectic or eutectoid structures as an effective phase region when using the ‘unresolved’ nucleation option was essentially improved and is now consistent with FD correction,

small grain treatment, averaging of driving forces, etc. The according output was adjusted as illustrated in the new example 'A015_AlSiMg_Unresolved.dri'.

- Extra updates of thermodynamic data in global relinearisation modes: In global relinearisation modes (global, globalF, globalG, globalGF), the linearised thermodynamic data is now automatically updated for fast moving interfaces (global, globalG) or fragments (globalF, globalGF). By now, new interface cells were only provided with a copy of the existing global relinearisation parameters.
- Recrystallization-Model: Unified handling of driving forces for equal and unequal phase interaction.
- Improved handling of grain boundary diffusion in triple junctions.
- Corrected handling of negative misorientation angles in 2D to evaluate special orientation relationships (aniso_special_orient).
- Improved calculation of solubility ranges in IONIC_LIQUID models.
- Improvement of accuracy: Changed pre-factor in anti-trapping model obtained from calibration to a value obtained by an analytical benchmark.
- An inaccuracy of the DSC-output (dH/dT) has been removed which produced unintended noise on the DSC signal.
- The treatment of small nuclei was improved.

Stress solver

- A further homogenization approach for stresses and strains in the diffuse interface region- named Reuss/Sachs model - is now available which corresponds to the model explained in "I. Steinbach, M. Apel, Physica D 217 (2006) 153-160". All three elastic models available in the MICRESS "elastic module" (Voigt/Taylor, Khachaturyan, Reuss/Sachs) can now systematically be addressed for uncoupled (stress_u1, stress_u2, stress_u3), coupled (stress_ce1, stress_ce2, stress_ce3), and mechano-chemically coupled (stress_mc1, stress_mc2, stress_mc3) applications.
- For all three homogenization models (Voigt/Tailer, Khachaturyan, Reuss/Sachs), coupling to diffusion of elements can now be selected ("stress_mc1", "stress_mc2", "stress_mc3"). The model includes concentration dependent local eigenstrains, stress-driven diffusion, and stress-dependent quasi-equilibrium conditions.

Improvements in output:

- The output option for concentration (out_conc) and concentration per phase (out_conc_phase) are enriched by a new option for the concentration type (atom_percent | weight_percent). This kind of output type is only taken into account if a thermodynamic database is used. If this option is not given, the type of concentration output is fixed by the choice of the concentration input type.
- When calculating volume data from the database for the stress solver, an additional text output (.volD) is created which shows the molar volumes and their derivatives with respect to temperature and composition.
- The output of the default major compositions of the phases obtained from the TQ is complemented by the corresponding solubility range including user-defined limits.

- A new tabulated output for the volume-change model is available in the file volumetric data with extension "*TabVol".
- Additional output of molar phase fractions is generated in output *TabFrac in case of using the option 'volume change'.
- The .TabC output has been reconfigured by removing the minimum and maximum concentration information and by adding the compositions of the matrix element. Readability is strongly enhanced.

Improved performance:

A number of measures have been taken to improve performance e. g.:

- The time step criterion for grain boundary diffusion was reformulated, allowing for larger time steps.

Examples:

The number of examples included in the MICRESS® distribution again has been increased while some old examples have been updated and improved. Examples are classified into “application”, “training” and “benchmark” type examples to help users selecting an appropriate starting point for their work.

News on DP_MICRESS:

The post-processor DP_MICRESS brings the following new functionalities:

- Contour lines can be exported as tabular text files (Contour line dialog: File->Save Isolines)
- Open result dialog: new result types, i.e. mole, molV, expa, stiff, sigma, added to file filter
- Prototype functionality for a VTK export of a 2D projection of a 3D result
- Label orientations for the color scale bars can be switched between horizontal and vertical.
- Additional color scales, e.g. a cyclic scale for the representation of grain orientations.

News on MICpad:

MICpad allows for editing driving files. Bookmarks, colored comments and input strings largely facilitate navigating and editing especially large driving files. MICpad further acts as a control center allowing starting (locally) and monitoring the simulations as well as monitoring and organizing the results. The new features in MICpad 7.0 comprise:

Look and Feel:

- Layout changes: Results are displayed next to the driving file. Especially, the comparison between the .in file and the original driving file is much easier this way.
- The result list is reduced to the file extensions to enhance visibility.

New functionalities:

- Conversion of input format of driving files from MICRESS® Version 6.4 to MICRESS® version 7.0
- Driving file syntax parsing in the background is now possible. This allows for more robust parameter detection for tools like phase diagram plot, as only the real parameters play a role.
- Individual run configuration for each driving file
- Simulations can be suspended and continued.

News on AixViPMaP®:

The new AixViPMaP® simulation platform focuses on enabling automatic simulation workflows in the area of microstructure evolution and microstructure property relationships by continuum models. An article named : "AixViPMaP® - an operational platform for microstructure modelling workflows" and being authored by L. Koschmieder, S. Hojda, M. Apel, R. Altenfeld, Y. Bami, C. Haase, M. Lin, A. Vuppala, G. Hirt, and G.J. Schmitz has recently been published in: „Integrating Materials and Manufacturing Innovation" (open access download here). It presents and discusses three generic workflow examples which demonstrate the platform operation and which can be used as starting points for own applications. The AixViPMaP® platform framework is open-source and available for free. It can be downloaded from https://github.com/aixvipmap (accessed Nov 29th 2019). Consultancy in the installation and basic usage of the platform will be offered to MICRESS® customers by ACCESS e.V. AixViPMaP® and the AixViPMaP® logo are trademarks of ACCESS e.V..

Documentation:

The distribution of MICRESS® 7.0 for the first time has a full-online documentation, which can be accessed via the documentation tab on the MICRESS website or by calling the help function in either MICpad or DP_MICRESS.

We do hope that all these improvements will assist you in solving your problems and will continue to make MICRESS® a valuable tool for your research. For more details, please don't hesitate to ask us, preferentially via the MICRESS®-Forum (www.micress.de/forum). As a service for our customers we compiled all publications being related to the use of MICRESS® we became aware of since the last release in the appendix. Please notify us about your own publications to allow their inclusion as a reference into our website.

Yours sincerely
ACCESS e.V.

Dr. Georg J. Schmitz
Global Marketing, Sales & Support MICRESS®

Appendix: Recent publications related to MICRESS:

The following section provides a selection of recent (since last release) publications using MICRESS® and its features and/or the software ecosystem being built around MICRESS®. These articles provide some impressions about state of the art MICRESS simulations being performed by our customers and current topics being investigated using MICRESS®:

Chuanqi Zhu, Yuichiro Koizumi, Akihiko Chiba, Koretaka Yuge, Kyosuke Kishidad, Haruyuki Inuid
Pattern formation mechanism of directionally-solidified MoSi2/Mo5Si3 eutectic by phase-field simulation
Intermetallics; Volume 116, January 2020, 106590

L. Koschmieder, S. Hojda, M. Apel, R. Altenfeld, Y. Bami, C. Haase, A. Vuppala, G. Hirt, G.J. Schmitz
AixViPMaP® -an operational platform for microstructure modelling workflows; Integrating Materials and Manufacturing Innovation (2019) 8:122–143 https://doi.org/10.1007/s40192-019-00138-3

G.J. Schmitz: Materials Modelling: past, present, future (in German), RWTH Themen 1(2019) 8-15

G.J. Schmitz: Materials in an ICME framework: From composition and processing of materials to properties and applications of components, Proceedings NAFEMS World Congress 2019 Quebec, Kanada

G.J. Schmitz, G. Goldbeck, E. Ghedini, A. Hashibon, J. Friis: Towards an ICME Methodology in Europe – Nomenclature, Taxonomies, Ontologies, and Marketplaces, Proceedings NAFEMS World Congress 2019 Quebec, Kanada

G. Goldbeck, E. Ghedini, A. Hashibon, G.J. Schmitz, J. Friis: A Reference Language and Ontology for Materials Modelling and Interoperability; Proceedings NAFEMS World Congress 2019 Quebec, Kanada

A. Nicholas Grundy, S. Münch, S. Feldhaus, U. Hecht, J. Bratberg: Continuous Casting of High Carbon Steel: How Does Hard Cooling Influence Solidification, Micro-and Macro Segregation? IOP Conf. Series : Materials Science and Engineering 529 (2019) 012069 https://doi.org/10.1088/1757-899X/529/1/012069

G. Boussinot, M. Apel, J. Zielinski, U. Hecht, J.H. Schleifenbaum: Strongly Out-of-Equilibrium Columnar Solidification During Laser Powder-Bed Fusion in Additive Manufacturing Physical Review Applied. 11. (2019) https://doi.org/10.1103/PhysRevApplied.11.014025

C. Kumara, A. Segerstark, F. Hanning, N. Dixit, S. Joshi, P. Nylen and J. J. Moverare
Microstructure modelling of laser metal powder directed energy deposition of Alloy 718
Additive Manufacturing; Volume 25, January 2019, Pages 357-364
https://doi.org/10.1016/j.addma.2018.11.024

B. Böttger, B. Daniels, L. Dankl, T. Göhler, T. Jokisch
Systematic Phase-Field Study on Microstructure Formation During Brazing of Mar-M247 with a Si-Based AMS4782 Filler; Metallurgical and Materials Transactions A (2019) Pages 1-16
https://doi.org/10.1007/s11661-019-05113-3

Na Ta, Lijun Zhang, Yong Du
A trial to desgin γ / γ' bond coat in Ni-Al-Cr mode TCBs aided by phase-field simulation

Coatings 8 12 (2018) Pages 421-440, https://doi.org/10.3390/coatings8120421

G. Agarwal, A. Kumar, H. Gao, M. Amirthalingam, S.C. Moon, R.J. Dippenaar, I.M. Richardson, and M.J.M. Hermans: Study of Solidification Cracking in a Transformation-Induced Plasticity-Aided Steel Metallurgical and Materials Transactions A; Volume 49, April 2018, Pages 1015-1020 https://doi.org/10.1007/s11661-018-4505-7

B. Böttger, R. Altenfeld. G. Laschet, G. J. Schmitz, B. Stöhr, B. Burbaum
An ICME Process Chain for Diffusion Brazing of Alloy 247
Integrating Materials and Manufacturing Innovation 7 2 (2018) Pages 70-85
https://doi.org/10.1007/s40192-018-0111-1

Ming Wei, Lijun Zhang, Mingjun Yang, Kai Li, Shuhong Liu, Pizhi Zhao, Yong Du
Phase-field simulation of the solidified microstructure in a new commercial 6xxx aluminum alloy ingot supported by experimental measurements: Int. J. Mater. Res. (formerly Z. Metallkd.) 109 (2018) 2 , Pages 91-98 https://doi.org/10.3139/146.111584